Perfluorotriethylamine

	•			
359-70-6	DTXSID401894	16		

Model Performance

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.81	0.55	0.81	0.54	0.71	0.61	

Model Results

Predicted value: 2680 L/kg

Global applicability domain: Outside

Local applicability domain index: 1.39e-01

Confidence level: 7.15e-01

Nearest Neighbors from the Training Set

Image not found

Fthalide

Measured: 2000 Predicted: 1600 Image not found

Tridiphane

Measured: 5620 Predicted: 6630 Image not found

Chlorothalonil

Measured: 1820 Predicted: 1300

Image not found

3,4,5,6-Tetrachloroguaiacol

Measured: 708 Predicted: 685 Image not found

Pentachloronitrobenzene

Measured: 9550 Predicted: 10500